(2)

EDGEWOOD
RESEARCH,
DEVELOPMENT &
ENGINEERING
CENTER

ERDEC-TR-099

AD-A272 440

METHOD FOR DESIGN ROTATION

Ronald B. Crosier

RESEARCH AND TECHNOLOGY DIRECTORATE

August 1993

Approved for public release; distribution is unlimited.

U.S. ARMY
CHEMICAL
AND BIOLOGICAL
DEFENSE AGENCY

Aberdeen Proving Ground, Maryland 21010-5423

93-27696

3

Disclaimer

The findings in this report are not to be construed as an official Department of the Army position unless so designated by other authorizing documents.

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY *(Leave blank)*

2. REPORT DATE
1993 August

3. REPORT TYPE AND DATES COVERED
Final, 91 Dec - 92 Jun

4. TITLE AND SUBTITLE
Method for Design Rotation

5. FUNDING NUMBERS
PR-10161102A71A

6. AUTHOR(S)
Crosier, Ronald B.

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
DIR, ERDEC,* ATTN: SCBRD-RTM, APG, MD 21010-5423

8. PERFORMING ORGANIZATION REPORT NUMBER
ERDEC-TR-099

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES
*When this study was conducted, ERDEC was known as the U.S. Army Chemical Research, Development and Engineering Center, and the author was assigned to the Research Directorate.

12a. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution is unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

All rotations of a response surface design can be obtained by making planar rotations in the set of planes defined by every pair of the coordinate axes. Standard multivariate optimization routines may then be used to optimize a criterion for the desirability of a rotation as a function of the set of planar angles. Criteria for the symmetry of the design (such as the same set of factor levels for all factors) and for the size of the design region (changed by rescaling after the rotation) are developed. The hexagon design, the two-factor central composite design, the four-factor complex number design of Hardin and Sloan (1992), and the eight-factor uniform shell design are rotated to obtain a larger region, a symmetric treatment of the factors, or both.

14. SUBJECT TERMS
Orthogonal matrix
Uniform shell design
Complex number design
Response surface design
Central composite design
Multivariate optimization

15. NUMBER OF PAGES
27

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

Blank

PREFACE

The work described in this report was authorized under Project No. 10161102A71A, Research in CW/CB Defense. This work was started in December 1991 and completed in June 1992.

The use of trade names or manufacturers' names in this report does not constitute an official endorsement of any commercial products. This report may not be cited for purposes of advertisement.

This report has been approved for release to the public. Registered users should request additional copies from the Defense Technical Information Center; unregistered users should direct such requests to the National Technical Information Service.

Acknowledgments

The author thanks Alice M. Harper for many discussions during this work and for a review of the manuscript, James M. Lucas for comments on the manuscript, and the anonymous reviewers of *Technometrics* for their suggestions to improve the clarity of the manuscript.

Blank

CONTENTS

LIST OF FIGURES

LIST OF TABLES

METHOD FOR DESIGN ROTATION

1. INTRODUCTION

Response surface designs are used to develop a polynomial model relating a dependent variable y to a set of quantitative independent variables $x_1, x_2, \ldots, x_k$. Each row of the $N \times k$ design matrix $\mathbf{X}$ is a point in k-dimensional space. The dependent variable y is measured at each of the design points and the coefficients of the polynomial model are estimated from the data by the least-squares formula

$$\mathbf{b} = (\mathbf{M}'\mathbf{M})^{-1}\mathbf{M}'\mathbf{y}, \tag{1}$$

where $\mathbf{b}$ is the estimated coefficient vector and $\mathbf{M}$ is the $N \times p$ expanded design matrix, or model matrix, that has one column for each coefficient of the polynomial model.

Many designs have been proposed for the estimation of the coefficients of first- and second-degree polynomial models. The designs are centered at the origin and scaled so that the design levels are convenient numbers—such as integers, simple fractions, and their square roots; a change of origin and scale makes the designs applicable to applied problems. Because a response surface design is a set of points in k-dimensional space, a rotation of the coordinate axes will produce a new design matrix that represents the same geometric figure as the original design. An elementary result in linear algebra is that multiplication by an orthogonal matrix $\mathbf{P}$ corresponds to a rotation of the coordinate axes if the determinant of $\mathbf{P}$ is 1, and to a rotation followed by a reflection—a change of sign or direction of one axis—if the determinant of $\mathbf{P}$ is -1. Hence there is no theoretical problem in obtaining rotations of a design; there are only the practical questions Why rotate a design? And how can a useful orthogonal matrix be selected to rotate the design?

2. MOTIVATION

The well known D- and G-efficiencies of first- and second-order response surface designs are not affected by a rotation of the coordinate axes—see the proof in the Appendix. One must look at other criteria to see any benefit from design rotation. Two criteria examined here are the size of the design region and the symmetry of the design matrix. The starting point for the theory of response

surface designs is the specification of the design region; it is usually taken to be a cube or sphere of a specified size (in coded units). For spherical designs, the ranges of the coded design factors are not considered important, and designs are compared by scaling them to the same diameter. In this report, I take a different approach to developing a response surface design.

Suppose an experimenter wishes to vary cooking time from 40 to 60 minutes, and cooking temperature from 180 to 200 degrees. I assume that, regardless of the design used, the range of the coded design factors must be scaled to the ranges of the experimental factors so that cooking time varies from 40 to 60 minutes, and temperature varies from 180 to 200 degrees. Such a scaling of the coded design factors to the experimental factors is necessary to give the experimenter a design with the specified ranges.

The specification of ranges for the experimental factors does not imply a cuboidal region. The midpoints of the ranges of the experimental factors usually represent the current process settings or a guess of the factor settings that will optimize y. The exploration of the region around the center point of the design should be symmetrical (that is, a spherical design) unless the experimenter specifies that some directions are more important than others. A cuboidal region would be appropriate, for example, if the experimenter specifies that the directions toward the corners of the cube are more important than the directions toward the centers of the faces of the cube.

Two examples will show how the size of the design region and symmetry of design matrix can be changed by a rotation of the design. The first example involves a rotation and scaling of the central composite design for two factors. The central composite designs were developed by Box and Wilson (1951) and consist of (a) center points at the origin, (b) axial or star points, which can be represented in a shorthand notation by the permutations of $(\pm 1, 0, \cdots, 0)$, and (c) factorial points, which are a two-level factorial or fractional factorial design of at least resolution V and can be represented by $(\pm\alpha^{-1}, \pm\alpha^{-1}, \cdots, \pm\alpha^{-1})$. Typical choices for α are the square root of k, which places the noncentral design points on the surface of a sphere, and the fourth root of the number of factorial points, which makes the contours of constant prediction variance spherical. Figure 1 shows a rotation and scaling of the two-factor central composite design. The effect of the rotation and scaling is to make the design cover a larger region (the large outer circle in Fig. 1) when the rotations are scaled to cover the same range. Table 1 gives the coded design settings of the central composite design, the rotated design,

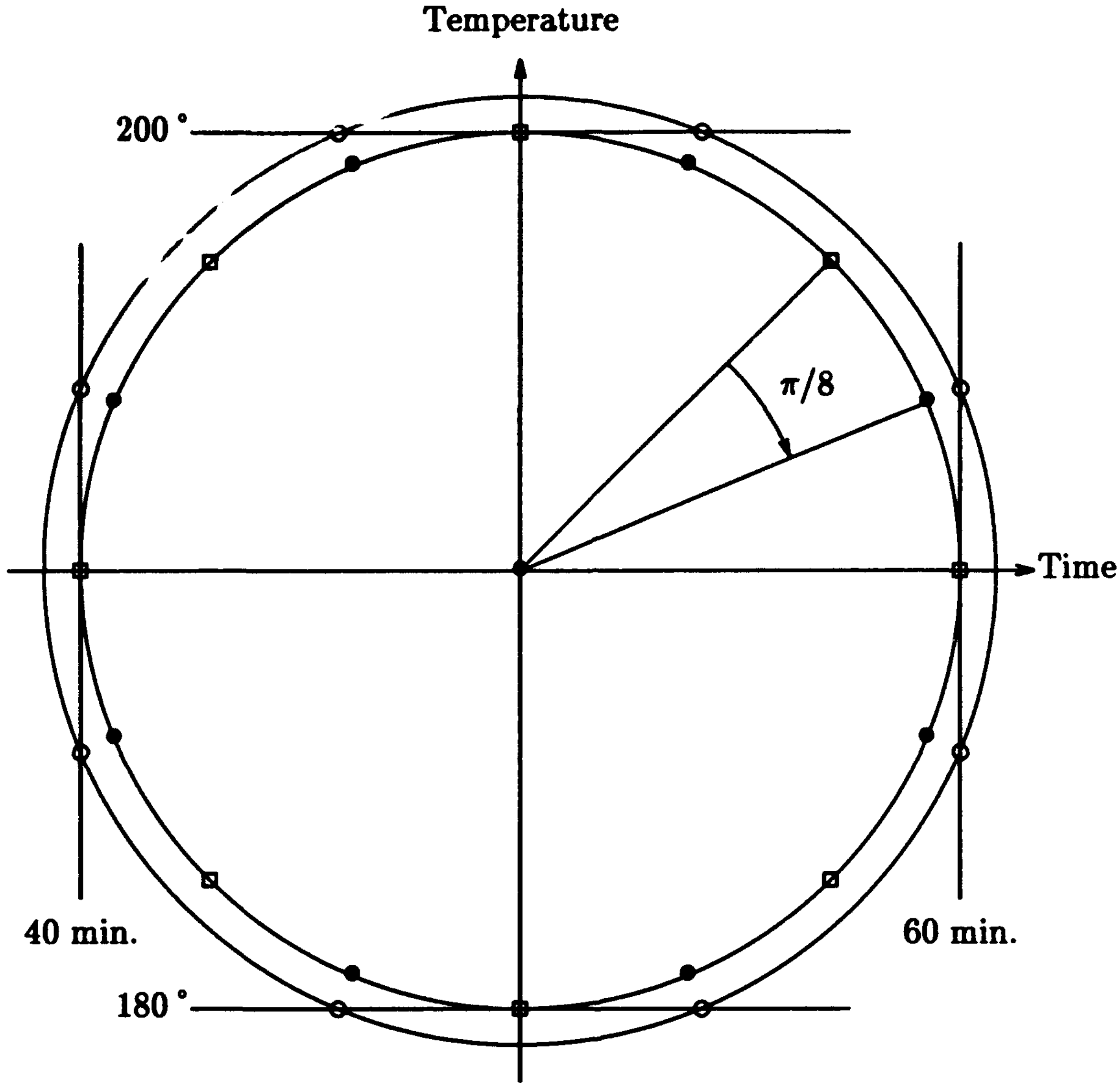

Figure 1. A Rotation and Scaling of the Two-Factor Central Composite Design. The design points before rotation are indicated by small squares. The design is first rotated (solid dots), then scaled to cover the same range as the design before rotation (hollow dots).

---

and the rotated and scaled design. The advantage of the larger region of the rotated and scaled design is that it gives a better estimates of the model coefficients when the designs are applied in the usual manner. Table 2 shows that the larger experimental region of the rotated and scaled design in Table 1 yields better

Table 1. Two Factor Central Composite Design

Point	Coordinates x_1	x_2	...Rotated w_1	w_2	...and Scaled x_1	x_2	Block
1	−.707	−.707	−.924	−.383	−1.	−.414	1
2	.707	−.707	.383	−.924	.414	−1.	1
3	−.707	.707	−.383	.924	−.414	1.	1
4	.707	.707	.924	.383	1.	.414	1
5	0.	0.	0.	0.	0.	0.	1
6	−1.	0.	−.924	.383	−1.	.414	2
7	1.	0.	.924	−.383	1.	−.414	2
8	0.	−1.	−.383	−.924	−.414	−1.	2
9	0.	1.	.383	.924	.414	1.	2
10	0.	0.	0.	0.	0.	0.	2

Table 2. Variance of Estimated Coefficients

Model Term	Standard Orientation	Rotated and Scaled
constant	.5 σ^2	.5 σ^2
linear	.25 σ^2	.213 σ^2
quadratic	.875 σ^2	.637 σ^2
interaction	1.0 σ^2	.729 σ^2

estimates of the model coefficients. Scaling the design to cover the larger region increases the determinant of **M′M** from 256 to 909.

The second example is a rotation and scaling of the hexagon design. Table 3 gives the coordinates of the design both before and after the rotation and scaling; Figure 2 shows the rotation and scaling.

Table 3. Hexagon Design

Point	Coordinates x_1	x_2	Rotated and Scaled x_1	x_2	Block
1	1.	0.	1.	−.268	1
2	−.5	.866	−.268	1.	1
3	−.5	−.866	−.732	−.732	1
4	0.	0.	0.	0.	1
5	−1.	0.	−1.	.268	2
6	.5	−.866	.268	−1.	2
7	.5	.866	.732	.732	2
8	0.	0.	0.	0.	2

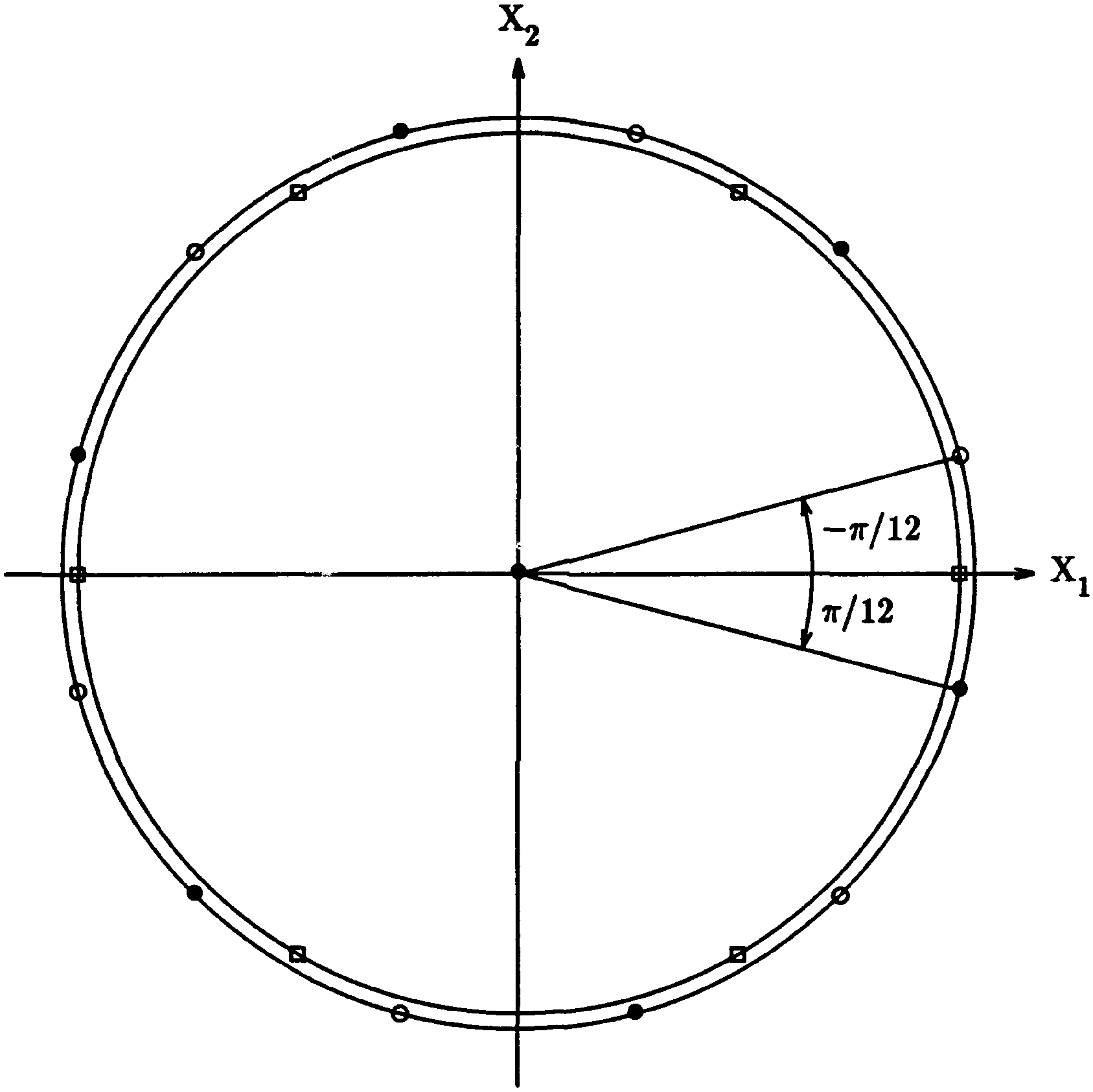

Figure 2. Two Rotations and Scalings of the Hexagon Design. The hexagon design in its usual orientation is indicated by small squares. After rotation by $\pi/12$ radians and scaling the factor levels to the range -1 to 1, the design points are indicated by a solid dots for a clockwise rotation of the design and by hollow dots for a counterclockwise rotation of the design. Notice that the clockwise and counterclockwise rotations are reflections across the x_1-axis; multiplying the second coordinate by -1 will change one rotation into the other.

In the standard orientation of the hexagon design, the first factor covers the

interval $(-1,1)$ and the second factor covers the interval $(-.866,.866)$. In the new orientations, both factors cover the interval $(-1,1)$; the rotated designs also cover a slightly larger region than the original design.

The unequal ranges of the factors of the hexagon design in its usual orientation create a problem in applying the design. If the levels $-.866$ and $.866$ of the second factor are scaled to 180 and 200 degrees for the two-factor cooking example, then the design is no longer a spherical design, but an ellipsoidal design based on an irregular hexagon. This method of applying the design essentially ignores the levels $-.866$ and $.866$ of the second factor; they could be replaced by -1 and 1 without affecting the levels of cooking temperature used by the experimenter.

An alternative method of applying the design is to associate the diameter of the circle with the ranges of the experimental factors. The design diameter of two units would therefore correspond to the full range of cooking temperature (180 to 200 degrees). Because the second design factor varies from $-.866$ to $.866$, cooking temperature would be varied from 181.3 degrees to 198.7 degrees in the experiment. This latter method of applying the design is consistent with the theory of optimal designs, but tends to produce counter-productive consultant-client discussions.

The new orientations of the hexagon design give both factors the range -1 to 1, so they do not create a problem in associating the range of the coded design factors to the ranges of the experimental factors. The price paid for the symmetric orientations of the hexagon design is that the design now has seven levels of each factor. An alternative is to use the central composite design, which has only five levels, but requires more experimental runs.

These examples suggest that both the practical efficiency and the correctness of application (or the client-friendliness) of a response surface design may be affected by a rotation of the design. So how can desirable rotations be obtained? There is little information in the literature on design rotation. Box and Behnken (1960) note that their four-factor design is a rotation of the four-factor central composite design and give the orthogonal matrix that yields the rotation, but they do not discuss how the orthogonal matrix was found.

Doehlert and Klee (1972) gave rotations of Doehlert's (1970) uniform shell designs that minimize the number of levels of the factors. A technique used by Doehlert and Klee (1972) was to start with a known orthogonal matrix of simple form and then augment the matrix with additional rows and columns to get a

matrix that yields the minimum number of factor levels for the next higher dimensional design. The augmentation process can be applied to other sequences of designs, but a useful orthogonal matrix is required to start the process. Crosier (1991) gave symmetric orientations of response surface designs for mixture experiments. No orthogonal matrices were given, although there must be matrices that map, for example, the three-dimensional central composite design to the mixture space for four components.

In summary, the existing literature provides little guidance for rotating response surface designs. The only helpful idea is to augment an orthogonal matrix to serve the next higher dimension in a sequence of designs that have the same construction. The development of useful orthogonal matrices to start the process is an intuitive process. The numerical techniques developed in this report are offered as a supplement to the intuitive approach to obtaining design rotations. Neither approach is guaranteed to find the best solution. Doehlert and Klee (1972), for example, missed the five-level orientation of the eight-factor uniform shell design given in Table 4. The design in Table 4 can be orthogonally blocked: the points in Table 4 are one block and their negatives are the other block; the same number of center points must be used with each block. The design in Table 4 is one design in the class of uniform shell designs; the symmetric orientation of the uniform shell designs was found using the numerical techniques described in the next section.

3. AN APPROACH TO DESIGN ROTATION

3.1 Parameterization of Orthogonal Matrices

The rotation of a response surface design can be written in matrix notation as

$$\mathbf{W} = \mathbf{X}\,\mathbf{G} \tag{2}$$

where $\mathbf{W}$ is the rotated design matrix, $\mathbf{X}$ is the $N \times k$ design matrix, and $\mathbf{G}$ is a $k \times k$ orthogonal matrix whose determinant is one.

To optimize some criterion for $\mathbf{W}$ as a function of $\mathbf{G}$, it is necessary to parameterize $\mathbf{G}$ as a vector $\boldsymbol{\theta}$ whose elements can be varied independently of each other. The k^2 elements of $\mathbf{G}$ cannot be varied independently because $\mathbf{G}$ must remain an orthogonal matrix. $\mathbf{G}$ can be expressed as the product of $k(k-1)/2$

Table 4. Rotated Eight-Factor Uniform Shell Design

Point	x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8
1	−1.	1.	0.	0.	0.	0.	0.	0.
2	0.	−1.	1.	0.	0.	0.	0.	0.
3	0.	0.	−1.	1.	0.	0.	0.	0.
4	0.	0.	0.	−1.	1.	0.	0.	0.
5	0.	0.	0.	0.	−1.	1.	0.	0.
6	0.	0.	0.	0.	0.	−1.	1.	0.
7	0.	0.	0.	0.	0.	0.	−1.	1.
8	1.	0.	0.	0.	0.	0.	0.	−1.
9	−1.	0.	1.	0.	0.	0.	0.	0.
10	0.	−1.	0.	1.	0.	0.	0.	0.
11	0.	0.	−1.	0.	1.	0.	0.	0.
12	0.	0.	0.	−1.	0.	1.	0.	0.
13	0.	0.	0.	0.	−1.	0.	1.	0.
14	0.	0.	0.	0.	0.	−1.	0.	1.
15	1.	0.	0.	0.	0.	0.	−1.	0.
16	0.	1.	0.	0.	0.	0.	0.	−1.
17	−1.	0.	0.	1.	0.	0.	0.	0.
18	0.	−1.	0.	0.	1.	0.	0.	0.
19	0.	0.	−1.	0.	0.	1.	0.	0.
20	0.	0.	0.	−1.	0.	0.	1.	0.
21	0.	0.	0.	0.	−1.	0.	0.	1.
22	1.	0.	0.	0.	0.	−1.	0.	0.
23	0.	1.	0.	0.	0.	0.	−1.	0.
24	0.	0.	1.	0.	0.	0.	0.	−1.
25	−1.	0.	0.	0.	1.	0.	0.	0.
26	0.	−1.	0.	0.	0.	1.	0.	0.
27	0.	0.	−1.	0.	0.	0.	1.	0.
28	0.	0.	0.	−1.	0.	0.	0.	1.
29	.5	−.5	−.5	−.5	−.5	−.5	−.5	−.5
30	−.5	.5	−.5	−.5	−.5	−.5	−.5	−.5
31	−.5	−.5	.5	−.5	−.5	−.5	−.5	−.5
32	−.5	−.5	−.5	.5	−.5	−.5	−.5	−.5
33	.5	.5	.5	.5	−.5	.5	.5	.5
34	.5	.5	.5	.5	.5	−.5	.5	.5
35	.5	.5	.5	.5	.5	.5	−.5	.5
36	.5	.5	.5	.5	.5	.5	.5	−.5

NOTE: Add negatives and center points.

matrices, each of which represents a rotation in a plane defined by two coordinate axes. All pairs of axes are included in this factorization of G, which can be written

$$\mathbf{G} = (\mathbf{G}_{12}\mathbf{G}_{13} \cdots \mathbf{G}_{1k})(\mathbf{G}_{23} \cdots \mathbf{G}_{2k}) \cdots (\mathbf{G}_{k-1,k}), \tag{3}$$

where the matrix $\mathbf{G}_{ij}$ is formed by replacing four elements of a $k \times k$ identity matrix;

the i,i and j,j elements are $cos(\theta_{ij})$, the i,j element is $-sin(\theta_{ij})$ and the j,i element is $sin(\theta_{ij})$. The $\mathbf{G}_{ij}$ matrices represent a clockwise rotation of the design—that is, the design is rotated from the positive x_j axis toward the positive x_i axis. The representation of the matrix **G** as the product of $k(k-1)/2$ matrices is a useful conceptual tool, but it is not necessary to actually form and multiply all the $\mathbf{G}_{ij}$'s to obtain **G**. **G** can be obtained from an identity matrix in $k(k-1)/2$ stages that require only a linear transform of two columns; each stage corresponds to post-multiplication by a $\mathbf{G}_{ij}$ matrix. Post-multiplication by $\mathbf{G}_{ij}$ transforms the ith and jth columns by the equations

$$g^*_{ni} = cos(\theta_{ij})\, g_{ni} + sin(\theta_{ij})\, g_{nj} \tag{4}$$

and

$$g^*_{nj} = -sin(\theta_{ij})\, g_{ni} + cos(\theta_{ij})\, g_{nj} \tag{5}$$

where $n=1,2,\ldots,k$ is the row index and g^*_{ni} and g^*_{nj} are the values in the ith and jth columns after the transformation. In programming equations (4) and (5), it is necessary to put the value of g^*_{ni} into a temporary storage location so that g_{ni} is still available when equation (5) is implemented; it is also customary to take the calculation of $cos(\theta_{ij})$ and $sin(\theta_{ij})$ outside the loop over the rows of **G**.

Because **G** is an orthogonal matrix with determinant 1, equation (2) does not allow for rotations followed by a reflection. Sign changes of the factors do not affect the criteria proposed below for the desirability of a rotation. Hence, the method developed in this section is able to find a good rotation of a design, although it may be necessary to change the sign of a factor to put the rotated design in a convenient form.

3.2 Criteria for Selecting a Rotation

The examples in Section 2 show what properties of a design may be changed by rotation and therefore what criteria need to be specified for the objective function of the multivariate optimization procedure. Rotating a design does not change its diameter, so the range of the coded factors is used to measure the size of the design. As can be seen in Table 1, rotation of a design should *minimize* the range of the coded factors so that rescaling the design will increase the size of the experimental region. Because most rotations are likely to have different ranges for

the factors, the largest range ($R_{\max}$) will be taken as the first criterion to be minimized.

The second example in Section 2 showed that equal ranges for the factors might be obtained by rotation. To obtain this goal, the difference between the largest and smallest range

$$\Delta R = R_{\max} - R_{\min} \tag{6}$$

may be minimized by the optimization procedure. The symmetric orientation of the uniform shell designs was found by using the sum of the two criteria $R_{\max}$ and ΔR as the objective function for the multivariate optimization. Although this success showed that these criteria could be effective, additional criteria were developed to indicate other properties of symmetric designs.

Design factors can have equal ranges without being defined over the same interval; for example, the first factor may cover the interval −1 to 2, whereas the second factor covers the interval −2 to 1. It is also possible that the factors may have the same range, but the range is asymmetric about zero, the center of the design. For example, the factors may all cover the interval −1 to 2, even though the design is centered at the origin. To develop a test for symmetric ranges, let L_j be the minimum value in the jth column of the rotated design matrix $\mathbf{W}$ and let H_j be the maximum value in the jth column of $\mathbf{W}$. A criterion for obtaining symmetric ranges is

$$R_{sym} = \sum_{j=1}^{k} | L_j + H_j | . \tag{7}$$

This criterion will be zero if $L_j = -H_j$ for $j = 1, 2, \ldots, k$—that is, if all the factors have symmetric ranges.

In addition to having the same, symmetric range for all factors, a symmetric design should have the same set of factor levels for all factors. An exact test for the same set of factor levels for all factors would be cumbersome, so the following indicator was developed to search for designs with the same set of levels for every factor. Find the sum of absolute values (SAV) of the factor levels for each factor; take the difference between the largest and smallest of these sums. The difference will be zero if the factors have the same set of levels. The quantity to be minimized by the optimization procedure is

$$\Delta SAV = \max_j \sum_{i=1}^{N} |w_{ij}| - \min_j \sum_{i=1}^{N} |w_{ij}|. \tag{8}$$

The criteria developed here are suggestive, not exhaustive. Criteria that capture better the ideas of symmetry and size might be developed and criteria that reflect other goals may certainly be used.

3.3 Random Starts for the Optimization Procedure

Multivariate optimization procedures often terminate at local optimum, rather than at the global optimum. Because of this phenomenon, it is customary to start the multivariate optimization procedure with many different initial guesses for the solution vector. A simple method of obtaining different initial values for the vector θ is to generate each θ_{ij} as a uniform random variate over the interval $(0, 2\pi)$. This method is adequate for practical purposes but it is subject to criticism on theoretical grounds. The columns (or rows) of G can be interpreted as points on the surface of a sphere of radius 1; the use of uniformly distributed θ_{ij}*'s* does not generate a sequence of random orthogonal matrices whose columns are uniformly distributed over a sphere. To obtain random orthogonal matrices whose columns represent points uniformly distributed over a sphere, it is necessary that the angles θ_{ij} have a distribution that depends on the value of $j-i$. Anderson, Olkin, and Underhill (1987) give the following method of obtaining the required angles.

Let $\theta_{ij} = \arccos(t_{j-i}^{1/2})$, where $t_{j-i} = \sum_{m=1}^{j-i} u_m \Big/ \sum_{m=1}^{j-i+1} u_m$

and the u*'s* are independent random chi-square variates with one degree of freedom. Anderson *et al* (1987) point out that after setting $t_1 = u_1/(u_1+u_2)$, it is possible to use the denominator of t_1 as the numerator in $t_2 = (u_1+u_2)/(u_1+u_2+u_3)$ because the properties of chi-square variates make t_1 and t_2 independent. Thus, for fixed i, the $k-i$ θ_{ij}*'s* can be created from $k-i+1$ independent chi-square variates.

4. EXAMPLE

Hardin and Sloane (1992) give a second-order response surface design for four factors in 16 runs by pairs of complex numbers. I call their design the complex number design. Table 5 gives the real-valued coordinates for the four factors of the

Table 5. The Complex Number Design

Point	x_1	x_2	x_3	x_4
1	0.	0.	0.	0.
2	1.	0.	0.	0.
3	−.5	.866	0.	0.
4	−.5	−.866	0.	0.
5	0.	0.	1.	0.
6	0.	0.	−.5	.866
7	0.	0.	−.5	−.866
8	−.707	0.	−.707	0.
9	−.707	0.	.354	−.612
10	−.707	0.	.354	.612
11	.354	−.612	−.707	0.
12	.354	−.612	.354	−.612
13	.354	−.612	.354	.612
14	.354	.612	−.707	0.
15	.354	.612	.354	−.612
16	.354	.612	.354	.612

complex number design. Rows 2-4 in Table 5 correspond to the pair of complex numbers $(\omega^r, 0)$ for $r=0$, 1, and 2, where $\omega = exp(2\pi i/3)$; rows 5-7 are $(0, \omega^r)$ for $r=0$, 1, 2; and rows 8-16 are $2^{-1/2}(-\omega^r, -\omega^s)$ for $r=0$, 1, 2 and $s=0$, 1, 2 at each value of r.

The design has been oriented to minimize the number of levels of the factors, but Hardin and Sloane (1992) do not discuss how this orientation was obtained. Notice that the first and third factors cover the interval −.707 to 1, whereas the second and fourth factors cover the interval −.866 to .866. The objectives in rotating this design were to obtain (a) a symmetric range for each factor, (b) the same range for each factor, (c) the same set of levels for each factor, and (d) a large region. It was not clear if all these objectives could be attained, nor was it clear how such objectives could be pursued without the method developed in this report.

The first step in exploring this problem was to generate 100 random θ's by the method of Anderson *et al* (1987). The criteria discussed in Section 3 were calculated for the 100 random orientations of the design given by this set of θ's. Table 6 gives the mean, standard deviation, minimum and maximum of the criteria for the 100 random orientations, for the design as initially given by Hardin and Sloane (1992), and for the optimized design. For the optimization, objective function was a weighted average of the four criteria; the weights were proportional to the reciprocals of the standard deviations of the criteria. Other methods of weighting the criteria could be used. For example, a different set of randomly

Table 6. Criteria for Rotations of the Complex Number Design

Criterion	100 Random Orientations Mean	St. Dev.	Min.	Max.	Initial	Optimized
R_{max}	1.78	.04	1.69	1.84	1.73	1.71
ΔR	.12	.05	.02	.25	.02	.00
R_{sym}	.40	.13	.07	.67	.59	.00
ΔSAV	.35	.18	.07	.81	.84	.00

varying weights could be used with each starting point $\boldsymbol{\theta}$.

The Nelder-Mead downhill simplex method, as described by Press, Flannery, Teukolsky, and Vetterling (1986), was used for the optimization. Again, this was merely a convenient choice; other optimization methods, such as direction-set methods, annealing methods (see Press *et al* 1986 for a description of these), or genetic algorithms (see Goldberg 1989) could be used. The 100 random $\boldsymbol{\theta}$'s were used as starting points for the optimization. From an initial point $\boldsymbol{\theta}_0$, the downhill simplex method creates a simplex by generating $m = k(k-1)/2$ additional points as follows. For $i = 1, 2, \ldots, m$, let $\boldsymbol{\theta}_i = \boldsymbol{\theta}_0 + \lambda \mathbf{e}_i$, where $\mathbf{e}_i$ is the elementary vector with a one in the ith place and zeros elsewhere. For the initial simplex, λ was set at three radians. The downhill simplex method moves the simplex away from the worst point and shrinks the simplex until the relative difference between the objective function at the best point and the objective function at the worst point reaches a predetermined value, or until a maximum number of iterations has been reached. The termination criterion was a relative tolerance of 10^{-7} in the objective function, or a limit of 500 iterations. Of the 100 optimizations, only 11 were terminated by the 500-iteration limit. The angles in the optimized $\boldsymbol{\theta}$'s, the design levels in **W**, and the four criteria for a design were generally accurate to two or three decimal places—as judged by the agreement between different optimizations that terminated at the same, or equivalent, rotations. A rerun of the optimizations, with the optimized $\boldsymbol{\theta}$'s as the starting points and $\lambda = .01$, added another decimal place of accuracy.

Two symmetric orientations were found that have the same value by each criterion. The two orientations, after scaling the factor levels to cover the interval -1 to 1, are given in Tables 7 and 8. The first orientation (Table 7) can be obtained by using $\boldsymbol{\theta}' = (5\pi/6, 3.486, 5.161, 3\pi/2, 2.299, 7\pi/4)$, changing the sign of the first factor, and scaling the design to the range -1 to 1. The second orientation (Table 8) can be obtained by using $\boldsymbol{\theta}' = (-\pi/6, 0, \arctan(2^{1/2}), \pi/2, 3\pi/4, \pi/4)$, changing the sign of the fourth factor, and scaling. The second orientation is

Table 7. A rotation of the Complex Number Design

Point	x_1	x_2	x_3	x_4
1	0	0	0	0
6	g	g	0	0
4	0	0	g	g
7	−1	b	−d	d
5	b	−1	d	−d
3	d	−d	−1	b
2	−d	d	b	−1
10	1	−d	b	d
11	−d	1	d	b
13	d	b	1	−d
8	b	d	−d	1
16	f	−a	−c	−h
14	−a	f	−h	−c
12	−h	−c	f	−a
9	−c	−h	−a	f
15	−e	−e	−e	−e

NOTE: $a=3/2^{1/2}-2\approx.121$
$b=2^{1/2}a\approx.172$
$c=1-2^{-1/2}\approx.293$
$d=2^{1/2}-1\approx.414$
$e=2-2^{1/2}\approx.586$
$f=2^{-1/2}\approx.707$
$g=2d\approx.828$
$h=3c\approx.879$

preferable to the first because it has an additional type of symmetry not found in the first orientation: if a factor occurs at level a, it also occurs at level $-a$.

5. ADDITIONAL TOPICS

5.1 Multiple Solutions

Any angle in θ may be replaced by $\theta_{ij}+2\pi$ without changing the rotated design. In addition to the multiple solutions created by the periodic nature of the sine and cosine functions, there are other solutions (θ's) that represent all permutations of the columns of $\mathbf{W}$ and usually some permutations of the rows of $\mathbf{W}$. The different row orders that can be obtained by rotation are called equivalent row orders; the implications of nonequivalent row orders are discussed in the next paragraph.

Table 8. Another Rotation of the Complex Number Design

Point	s_1	s_2	s_3	s_4
1	0	0	0	0
6	g	g	0	0
4	0	0	g	g
7	−g	0	e	−e
5	0	−g	−e	e
3	−e	e	−g	0
2	e	−e	0	−g
9	−1	−b	0	e
12	−b	−1	e	0
16	e	0	−1	−b
14	0	e	−b	−1
13	1	−d	b	d
8	−d	1	d	b
11	d	b	1	−d
10	b	d	−d	1
15	−e	−e	−e	−e

NOTE: *b, d, e,* and *g* are defined in Table 7.

5.2 Proving That Two Designs Are Rotations

It may be of interest to show that two $N \times k$ design matrices **A** and **B** are, or are not, rotations of each other. Applying the theory of generalized inverses to solve $\mathbf{A} = \mathbf{B}\mathbf{P}$ for **P**, with the idea of showing that **P** is an orthogonal matrix, yields $\mathbf{P} = (\mathbf{B}'\mathbf{B})^{-1}\mathbf{B}'\mathbf{A}$. But **P** may not be an orthogonal matrix even if one design is a rotation (or a rotation followed by a reflection) of the other. Nonequivalent row orders for **A** and **B** will make **P** a nonorthogonal matrix, even if **A** and **B** are rotations of each other.

5.3 The Shape of the Surface Over θ

If one considers the values of the objective function as a surface over the possible values of θ, then the shape of the surface depends not only on the objective function (the criteria used, and their weighting), but also on the orientation of the design in **X**. Multivariate optimization procedures are sensitive to the shape of the surface over the parameter space; some surfaces make the multivariate optimization problem easy, and others make the problem difficult. It is not known if the optimization process can be improved by updating the design in **X** whenever a better orientation is found.

5.4 Decomposition of P; Range of θ

Anderson *et al* (1987) give a method of decomposing an orthogonal matrix **P** into a set of angles θ that can be used to construct **G** and a diagonal matrix **D**; the diagonal matrix has 1's and −1's on the diagonal. Let $\mathbf{P}=\mathbf{GD}$; then $\mathbf{G}^{-1}\mathbf{P}=\mathbf{D}$. Because **G** is the product of $k(k-1)/2$ matrices, the decomposition of **P** into **D** and a set of angles is performed in $k(k-1)/2$ stages; each stage calculates θ_{ij} and then premultiplies **P** by $\mathbf{G}_{ij}^{-1}$. The θ_{ij}'s are extracted in the standard order (1,2), (1,3), ... (1,k), (2,3), etc. Let $\theta_{ij}=arctan(p_{ji}/p_{ii})$ if $p_{ii}>0$ and let $\theta_{ij}=\pi/2$ if $p_{ii}=0$. After extracting θ_{ij}, **P** is modified by using the equations

$$p^*_{in}=cos(\theta_{ij})\,p_{in}+sin(\theta_{ij})\,p_{jn} \tag{10}$$

and

$$p^*_{jn}=-sin(\theta_{ij})\,p_{in}+cos(\theta_{ij})\,p_{jn} \tag{11}$$

where $n=1,2,\ldots,k$ is the *column* index and p^*_{in} and p^*_{jn} are the values in the ith and jth *rows* after the transformation. Equations (10) and (11) are similar to equations (4) and (5) and can be programmed in a similar manner. At the end of the process **P** has been reduced to **D**.

The decomposition of **P** given by Anderson *et al* (1987) always yields angles θ_{ij} in the range $-\pi/2$ to $\pi/2$, whereas the angles in the multivariate optimization procedure are allowed to take on any value.

5.5 Test Cases and Results

For two factors, the rotations of the central composite design and of the hexagon design given in Section 2 may be used to test optimization routines and the programming of equations (4) and (5). For $k>2$ and k even, the central composite designs can be rotated to have a smaller range for the coded factors (and subsequently scaled to cover a larger region) by using $\theta_{ij}=\pi/4$ for i odd and $j=i+1$, and $\theta_{ij}=0$ otherwise.

Doehlert's (1970) uniform shell designs for $k>2$ can be rotated to give the factors equal ranges by using $\theta_{ij}=arcsin[(j-i+1)^{-1}]$ if $j<k$ and $\theta_{ij}=-arcsin[(j-i+1)^{-1/2}]$ if $j=k$. The designs produced by this rotation have

seven levels of the factors, except for the three-factor design (three levels—the Box-Behnken design) and the eight-factor design (five levels). It is necessary to change the sign of the last factor, as the preferred form for the new orientation is both a rotation and a reflection of the uniform shell designs. The designs for even k can be orthogonally blocked in the same manner as the design in Table 4.

6. SUMMARY

Figures illustrating rotations of the hexagon design and the octagon (or central composite) design showed how rotations can produce a symmetric treatment of the factors, a larger experimental region, or both. A rotation of the eight-factor uniform shell design (with levels -1, $-.5$, 0, .5, and 1 for each factor) was given.

Rotations of a response surface design can be obtained from standard multivariate optimization techniques. This method requires parameterization of orthogonal matrices by a set of parameters that can be varied independently and the specification of the objective function for the multivariate optimization routine. The factorization of an orthogonal matrix into matrices that represent planar rotations was used to represent the orthogonal matrix by a set of planar angles that can be varied independently. For the objective function, design criteria that represent the size of the design region and the symmetry of the design matrix were given. The specific criteria developed were the maximum range of the factors, the equality of the factor ranges, the symmetry of the factor ranges about the center point of the design, and the equality of the sets of factor levels.

Multivariate optimization procedures require a starting value (initial guess) for the vector of planar angles that represent an orthogonal matrix. The method of Anderson *et al* (1987) for generating the angles will produce a sequence of random orthogonal matrices that represent rotations uniformly distributed over a sphere.

The method for rotating a design was applied to the four-factor complex number design of Hardin and Sloane (1992). The criteria for the desirability of a rotation were calculated for 100 random orientations; the criteria were then divided by their standard deviations to form a weighted average for use as the objective function for the multivariate optimization. Two symmetric orientations of the design were found.

Appendix: Proof of Invariance of D- and G-Efficiency Under Rotation

The proofs for a second-order response surface design are more difficult than the proofs for a first-order model. I will give only the proofs for the second-order case in detail; the proofs for the first-order case are similar to those for the second-order case. These proofs show that the D- and G-efficiencies of a second-order response surface design are not changed by a rigid rotation of the coordinate axes. In a spherical region rotation of the coordinate axes is equivalent to a rotation of the design points. For a cuboidal region, rotation of the coordinate axes is equivalent to rotation of the design points and the cuboidal region simultaneously (so that the design points maintain the same relationship to the region boundaries as they had before the rotation).

Write the first- or second-order model as

$$\mathbf{y} = \mathbf{M}_x \beta + \epsilon \tag{A.1}$$

where $\mathbf{y}$ is the $N \times 1$ vector of responses, $\mathbf{M}_x$ is the $N \times p$ model matrix, β is the $p \times 1$ vector of coefficients, and ϵ is the $N \times 1$ vector of errors. A rotation (possibly followed by a reflection) of the $N \times k$ design matrix $\mathbf{X}$ is given by

$$\mathbf{W} = \mathbf{X}\mathbf{P}, \tag{A.2}$$

where $\mathbf{P}$ is an orthogonal matrix. The model matrix for the rotated design is $\mathbf{M}_w$ and the coefficient vector for the rotated design is denoted γ.

Let $\mathbf{M}_w = \mathbf{M}_x \mathbf{Q}$. For a first-order model,

$$\mathbf{Q} = \begin{bmatrix} 1 & \mathbf{0}' \\ \mathbf{0} & \mathbf{P} \end{bmatrix}. \tag{A.3}$$

$\mathbf{Q}$ is therefore an orthogonal matrix. For the second-order model the matrix that maps $\mathbf{M}_x$ to $\mathbf{M}_w$ is not an orthogonal matrix.

Reparameterize the model (1) for the second-order case by replacing the interaction (product) terms $x_i x_j$ by $2^{1/2} x_i x_j$ and the interaction parameters β_{ij} by $2^{-1/2} \beta_{ij}$. To write the reparameterized model in matrix notation, I introduce a diagonal matrix $\mathbf{C}$ that has 1's in the positions corresponding to the constant term, linear terms, and squared terms and $2^{1/2}$ in the positions corresponding to the

interaction terms. The reparameterized model is written

$$\mathbf{y} = \mathbf{M}_z\mathbf{C}\,\mathbf{C}^{-1}\beta + \epsilon. \tag{A.4}$$

After rotation of the design matrix $\mathbf{X}$ by $\mathbf{P}$, the model (4) becomes

$$\mathbf{y} = \mathbf{M}_w\mathbf{C}\,\mathbf{C}^{-1}\gamma + \epsilon. \tag{A.5}$$

For the reparameterized models,

$$\mathbf{M}_w\mathbf{C} = \mathbf{M}_z\mathbf{C}\,\mathbf{Q}, \tag{A.6}$$

where
$$\mathbf{Q} = \begin{bmatrix} 1 & \mathbf{0}' & \mathbf{0}' \\ \mathbf{0} & \mathbf{P} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{P}^{[2]} \end{bmatrix}.$$

$\mathbf{P}^{[2]}$ is the second Schlaflian matrix derived from $\mathbf{P}$ and maps the second-order terms of the reparameterized model to the second-order terms of the rotated, reparameterized model (see Box and Hunter 1957). $\mathbf{P}^{[2]}$ is an orthogonal matrix and therefore $\mathbf{Q}$ is also an orthogonal matrix.

To show the invariance of D-efficiency, I need to show that the determinant of $\mathbf{M}_w'\mathbf{M}_w$ is equal to the determinant of $\mathbf{M}_z'\mathbf{M}_z$. Using the elementary properties of matrices and determinants,

$$det[(\mathbf{M}_w\mathbf{C})'\,\mathbf{M}_w\mathbf{C}] = det(\mathbf{C}'\mathbf{M}_w'\mathbf{M}_w\mathbf{C}) = det(\mathbf{C}')\,det(\mathbf{M}_w'\mathbf{M}_w)\,det(\mathbf{C}). \tag{A.7}$$

Applying equation (A.6) to the left hand side of equation (A.7) gives

$$det[(\mathbf{M}_w\mathbf{C})'\,\mathbf{M}_w\mathbf{C}] = det[(\mathbf{M}_z\mathbf{C}\,\mathbf{Q})'\,\mathbf{M}_z\mathbf{C}\,\mathbf{Q}] = det(\mathbf{Q}'\mathbf{C}'\mathbf{M}_z'\mathbf{M}_z\mathbf{C}\,\mathbf{Q}) =$$

$$det(\mathbf{Q}')\,det(\mathbf{C}')\,det(\mathbf{M}_z'\mathbf{M}_z)\,det(\mathbf{C})\,det(\mathbf{Q}) = det(\mathbf{C}')\,det(\mathbf{M}_z'\mathbf{M}_z)\,det(\mathbf{C}) \tag{A.8}$$

because $det(\mathbf{Q}) = \pm 1$. Combining equations (A.7) and (A.8) gives

$$det(\mathbf{C}')\,det(\mathbf{M}_w'\mathbf{M}_w)\,det(\mathbf{C}) = det(\mathbf{C}')\,det(\mathbf{M}_z'\mathbf{M}_z)\,det(\mathbf{C}). \tag{A.9}$$

Because $det(\mathbf{C}) \neq 0$,

$$det(\mathbf{M}_w'\mathbf{M}_w) = det(\mathbf{M}_x'\mathbf{M}_x). \quad \text{(A.10)}$$

To show the invariance of G-efficiency under rotation, I need to show that the maximum prediction variance within the experimental region remains unchanged when the design is rotated. To do this, I will show that the prediction variance at every point in the region remains unchanged when the design is rotated. Let $\mathbf{x}'$ and $\mathbf{w}'$ be $1 \times p$ vectors that represent the same point in the models $\mathbf{M}_x$ and $\mathbf{M}_w$ respectively. In the reparametrized models using $\mathbf{M}_x\mathbf{C}$ and $\mathbf{M}_w\mathbf{C}$, the point is represented by $\mathbf{w}'\mathbf{C}$ and $\mathbf{x}'\mathbf{C}$, respectively. Therefore $\mathbf{w}'\mathbf{C} = \mathbf{x}'\mathbf{C}\mathbf{Q}$ and (its transpose) $\mathbf{C}'\mathbf{w} = \mathbf{Q}'\mathbf{C}'\mathbf{x}$.

Now examine the effect of the reparameterization on the prediction variance:

$$Var(\hat{y}\,|\,\mathbf{w}'\mathbf{C})/\sigma^2 = \mathbf{w}'\mathbf{C}[(\mathbf{M}_w\mathbf{C})'\mathbf{M}_w\mathbf{C}]^{-1}\mathbf{C}'\mathbf{w} = \mathbf{w}'\mathbf{C}[\mathbf{C}'\mathbf{M}_w'\mathbf{M}_w\mathbf{C}]^{-1}\mathbf{C}'\mathbf{w} =$$

$$\mathbf{w}'\mathbf{C}\,\mathbf{C}^{-1}(\mathbf{M}_w'\mathbf{M}_w)^{-1}\mathbf{C}'^{-1}\,\mathbf{C}'\mathbf{w} = \mathbf{w}'(\mathbf{M}_w'\mathbf{M}_w)^{-1}\mathbf{w} = Var(\hat{y}\,|\,\mathbf{w}')/\sigma^2. \quad \text{(A.11)}$$

Next, examine the effect of the rotation on the prediction variance of the reparameterized model:

$$Var(\hat{y}\,|\,\mathbf{w}'\mathbf{C})/\sigma^2 = \mathbf{w}'\mathbf{C}[(\mathbf{M}_w\mathbf{C})'\mathbf{M}_w\mathbf{C}]^{-1}\mathbf{C}'\mathbf{w} =$$

$$\mathbf{x}'\mathbf{C}\mathbf{Q}[(\mathbf{M}_x\mathbf{C}\mathbf{Q})'(\mathbf{M}_x\mathbf{C}\mathbf{Q})]^{-1}\mathbf{Q}'\mathbf{C}'\mathbf{x} = \mathbf{x}'\mathbf{C}\mathbf{Q}[\mathbf{Q}'\mathbf{C}'\mathbf{M}_x'\mathbf{M}_x\mathbf{C}\mathbf{Q}]^{-1}\mathbf{Q}'\mathbf{C}'\mathbf{x} =$$

$$\mathbf{x}'\mathbf{C}\mathbf{Q}\mathbf{Q}^{-1}\mathbf{C}^{-1}(\mathbf{M}_x'\mathbf{M}_x)^{-1}\mathbf{C}'^{-1}\mathbf{Q}'^{-1}\mathbf{Q}'\mathbf{C}'\mathbf{x} =$$

$$\mathbf{x}'(\mathbf{M}_x'\mathbf{M}_x)^{-1}\mathbf{x} = Var(\hat{y}\,|\,\mathbf{x}')/\sigma^2. \quad \text{(A.12)}$$

Combining equations (A.11) and (A.12) yields $Var(\hat{y}\,|\,\mathbf{w}') = Var(\hat{y}\,|\,\mathbf{x}')$.

APPENDIX

REFERENCES

Anderson, T. W., Olkin, I., and Underhill, L. G. (1987), "Generation of Random Orthogonal Matrices," SIAM *Journal on Scientific and Statistical Computing*, 8, 625-629.

Box, G. E. P., and Behnken, D. W. (1960), "Some New Three Level Designs for the Study of Quantitative Variables," *Technometrics*, 2, 455-475.

Box, G. E. P., and Hunter, J. S. (1957), "Multi-Factor Experimental Designs for Exploring Response Surfaces," *The Annals of Mathematical Statistics*, 28, 195-241.

Box, G. E. P., and Wilson, K. B. (1951), "On the Experimental Attainment of Optimum Conditions," *Journal of the Royal Statistical Society*, Ser. B, 13, 1-45.

Crosier, R. B. (1991), "Symmetry in Mixture Experiments," *Communications in Statistics— Theory and Methods*, 20, 1911-1935.

Doehlert, D. H. (1970), "Uniform Shell Designs," *Journal of the Royal Statistical Society*, Ser. C, 19, 231-239.

Doehlert, D. H., and Klee, V. L. (1972), "Experimental Designs Through Level Reduction of the d-Dimensional Cuboctahedron," *Discrete Mathematics*, 2, 309-334.

Goldberg, David E. (1989), *Genetic Algorithms in Search, Optimization, and Machine Learning*, Reading MA: Addison-Wesley.

Hardin, R. H. and Sloane, N. J. A. (1992), "Computer-Generated Minimal (and Larger) Response-Surface Designs: (I) The Sphere," Statistics Research Report, Room 2C-376, AT&T Bell Laboratories, 600 Mountain Avenue, Murray Hill, NJ 07974.

Press, W. H., Flannery, B. P., Teukolsky, S. A., and Vetterling, W. T. (1986), *Numerical Recipes: The Art of Scientific Computing*, Cambridge: Cambridge University Press.